A General Framework for Uncertainty Propagation Based on Point Estimate Methods

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ABSTRACT

A general framework to approach the challenge of uncertainty propagation in model based prognostics is presented in this work. It is shown how the so-called Point Estimate Methods (PEMs) are ideally suited for this purpose because of the following reasons: 1) A credible propagation and representation of Gaussian (normally distributed) uncertainty can be done with a minimum of computational effort for non-linear applications. 2) Also non-Gaussian uncertainties can be propagated by evaluating suitable transfer functions inherently. 3) Confidence intervals of simulation results can be derived which do not have to be symmetrically distributed around the mean value by applying PEM in conjunction with the Cornish-Fisher expansion. 4) Moreover, the entire probability function of simulation results can be reconstructed efficiently by the proposed framework. The joint evaluation of PEM with the Polynomial Chaos expansion methodology is likely to provide good approximation results. Thus, non-Gaussian probability density functions can be derived as well. 5) The presented framework of uncertainty propagation is derivative-free, i.e. even non-smooth (non-differentiable) propagation problems can be tackled in principle. 6) Although the PEM is sample-based the overall method is deterministic. Computational results are reproducible which might be important to safety critical applications. - Consequently, the proposed approach may play an essential part in contributing to render the prognostics and health management into a more credible process. A given study of a generic uncertainty propagation problem supports this issue illustratively.

This work includes unpublished elements of the Ph.D.-Thesis (Schenkendorf, 2014).

1. INTRODUCTION

Model based approaches in fault diagnosis and identification (FDI) have become quite popular in last decades. The value, however, of any derived mathematical model is directly linked to its predictive power. That is, to describe the essential features of interest as credibly as possible. In consequence of a potential model misspecification and measurement uncertainties the statistics of model based results has to be taken into account adequately. This is especially true in the field of prognostics and health management. For instance, the derived remaining useful life (RUL) of an analyzed device might suffer in its significance without any information of its credibility. The underlying problem of uncertainty propagation, however, is challenging for many real life applications. In this paper it is demonstrated how Point Estimate Methods (PEMs) are ideally suited to tackle the problem of uncertainty propagation efficiently, i.e. utilizing a minimum of computational effort but ensuring a good approximation power even for highly non-linear applications - which is usually the case in RUL calculation.

The remainder of this paper is organized as follows. In Section 2 the general problem of uncertainty propagation is addressed. In Section 3 the basics of the Point Estimate Methods are summarized. Moreover, it is discussed how non-Gaussian uncertainties can be considered in the PEM framework. Global sensitivities are addressed in 4. The proposed framework of uncertainty propagation is illustrated in Section 5. Finally, the conclusion is given in Section 6.

2. UNCERTAINTY PROPAGATION

The continuously rising number of articles devoted to problems of uncertainty propagation/management in the field of PHM (Saha, Goeble, Poll, & Christophersen, 2009; Daigle & Goebel, 2010; Daigle, Saxena, & Goebel, 2012; Lapira, Brisset, Davari, Siegel, & Lee, 2012; Williard, He, Osterman, & Pecht, 2013; Sankararaman & Goebel, 2013; Sankararaman, Daigle, Saxena, & Goebel, 2013; Daigle & Sankararaman, 2013; Kulkarni, Biswas, Celaya, & Goebel, 2013; X. Zhang & Pisu, 2014) is an excellent indicator for the significance of this topic but highlights that there are still unsolved issues to the same extent. Before introducing the PEM framework as

a versatile tool for uncertainty propagation, general problems in uncertainty propagation are briefly summarized.

To a certain extent, variability exists in any physical system. The uncertainty quantification as well as its adequate representation might be challenging in itself. Thus, to have a starting point only problems are going to be analyzed which act in the probabilistic framework exclusively. In general, the probability theory provides a comprehensive framework which, however, may suffer in practicability in the presence of nonlinearity. Consequently, there is a keen demand in a credible determination of probability density functions (PDFs) which are associated to computational results in PHM. The concepts of uncertainty propagation can be divided into analytical and in approximate methods, respectively. Analytical approaches might be suitable to illustrate the general concept of uncertainty propagation for deliberately chosen problems, but they suffer from practicability to the most real life applications.

2.1. Analytical Expressions

In general, the uncertainty propagation describes how a random variable, ξ, is transferred by a (non)-linear function, $g(\cdot)$, to the quantity of interest, η, according to

$$\eta = g(\xi) \tag{1}$$

Occasionally, ξ and η are referred to as the input and the output of an uncertainties propagation problem. For the purpose of readability, the proposed methodologies are introduced without loss of generality for 1-dimensional problems, i.e., $\xi \in \mathcal{R}^1$ and $\eta \in \mathcal{R}^1$. Additionally, unless otherwise specified, a standard Gaussian distribution of ξ is assumed, $\xi \sim \mathcal{N}(0,1)$. One possible way to represent the uncertainty about η consists in calculating the associated probability density function, pdf_η. Assuming a monotonic function, $g(\cdot)$, an analytical solution of the resulting PDF can be derived in principle (Breipohl, 1970; Hines, Montgomery, Goldsman, & Borror, 2003)

$$pdf_\eta = pdf_\xi\left(g^{-1}(\eta)\right)\left|\frac{dg^{-1}(\eta)}{d\eta}\right| \tag{2}$$

Any non-monotonic function has to be split up into monotonic sub-parts that are transferred separately (Breipohl, 1970; Hines et al., 2003).

Another point of interest might be in characteristic quantities of the associated PDF, i.e, statistical moments of pdf_η can be used as an alternative to characterize the induced uncertainty about η (Kay, 1993; Hines et al., 2003). For instance, the mean, $E\left[g(\xi)\right]$, and the related variance, σ_η^2, are frequently analyzed and can be determined by

$$E\left[g(\xi)\right] = \int_\Omega g(\xi) pdf_\xi d\xi \tag{3}$$

$$\sigma_\eta^2 = \int_\Omega \left[g(\xi) - E\left[g(\xi)\right]\right]^2 pdf_\xi d\xi \tag{4}$$

Here, Ω represents the integration domain, i.e., in case of probability theory it is equivalent to the sample space (Maitre & Knio, 2010). Throughout this work, also higher statistical moments are applied, e.g., the third, μ_3, and the fourth central moment, μ_4, are considered as well and expressed by

$$\mu_3 = \int_\Omega \left(g(\xi) - E\left[g(\xi)\right]\right)^3 pdf_\xi d\xi \tag{5}$$

$$\mu_4 = \int_\Omega \left(g(\xi) - E\left[g(\xi)\right]\right)^4 pdf_\xi d\xi \tag{6}$$

Unfortunately, the proposed analytical solutions of the PDF and/or statistical moments of η can be solved only for a limited number of uncertainty propagation problems (Breipohl, 1970; Stengel, 1994; Hines et al., 2003). In practice, however, approximate methods have to be applied. Here, the Taylor series expansion and sample-based approaches are of current interest and reviewed subsequently.

2.2. Basic Approaches in Approximate Methods

In real life, the complexity of $g(\cdot)$ - if at all available explicitly - prohibits results in closed-form. Consequently, approximate methods aim: (1) to replace $g(\cdot)$ by handy surrogate functions, $\hat{g}(\cdot)$, which facilitate closed-form solutions of Eq. (2)-(6). Or alternatively (2), to solve these integral expressions by numerical routines approximately.

2.2.1. Taylor Series Expansion

To solve equations similar to Eq. (2)-(6) in closed-form the mapping function, $g(\cdot)$, is approximated by a surrogate function, $\hat{g}(\cdot)$, first. Here, the most common approach is the Taylor series expansion. Under the assumption that $g(\cdot)$ is sufficiently differentiable, the uncertainty propagation function can be expressed by a superposition of Taylor terms:

$$\eta \approx \hat{g}(\xi) = \sum_{i=0}^{N} \left.\frac{\partial^i g}{\partial \xi^i}\right|_{\xi=E[\xi]} \frac{(\xi - E[\xi])^i}{i!} \tag{7}$$

Generally, this sum is limited to a certain extent, $N << \infty$, which may introduce an approximation error but ensures a manageable computation demand. In the field of uncertainty propagation, therefore, the first-order Taylor expansion can be considered as a standard approach with good reasons.

According to Eq. (1), the first-order Taylor series approximation is expanded at $\overline{\xi} = E[\xi]$ as shown below assuming without loss of generality a one-dimensional problem.

$$\eta \approx \hat{\eta} = g(\overline{\xi}) + \left.\frac{\partial g}{\partial \xi}\right|_{\xi=\overline{\xi}} (\xi - \overline{\xi}) \tag{8}$$

Here, the resulting function, $\hat{\eta}$, acts as a surrogate of the original function, η. Now, by evaluating $\hat{\eta}$ instead of η, the determination of statistical moments can be performed easily. For instance, the resulting mean $E[\hat{\eta}]$ is expressed by

$$E[\hat{\eta}] = g(E[\xi]) \tag{9}$$

In addition, the expectation of the squared difference of Eqs. (8) and (9) results into the variance expression of $\hat{\eta}$ according to

$$\sigma_{\hat{\eta}}^2 = \left(\left.\frac{\partial g}{\partial \xi}\right|_{\xi=\overline{\xi}} \right)^2 \sigma_{\xi}^2 \tag{10}$$

Obviously, the statistics about η is approximated by a linearization scheme and, therefore, only valid under serious constraints:

> "The Taylor series will be a good approximation if $g(\cdot)$ is not too far from linear within the region that is within one standard deviation of the mean."
>
> *A. M. Breipohl (Breipohl, 1970)*

Naturally, the utilization of higher-order terms in the Taylor series expansion improves the accuracy gradually. For instance, it has been shown that even an incorporation of a moderate number of higher-order terms leads to a significant improvement in accuracy (Xue & Ma, 2012), but ...

> "In practice, even the second order approximation is not commonly used and higher order approximations are almost never used."
>
> *U. N. Lerner (Lerner, 2002)*

The same is true, in case of non-Gaussian distributions and/or correlated random variables, see (Kay, 1993; J. Zhang, 2006; Mekid & Vaja, 2008; Anderson, 2011; Mattson, Anderson, Larson, & Fullwood, 2012) and references therein.

Additionally, the Taylor series is limited to problems of differentiable transfer functions, $g(\cdot)$. At first, that means, the transfer function has to be known explicitly. Therefore, black-box type functions cannot be addressed immediately. Secondly, even in case of explicit expressions, functions might be non-differential at all, e.g, the maximum function belongs to those terms. Hence, the Taylor series is likely to suffer in precision as well as in applicability.

3. POINT ESTIMATE METHODS

The method of Unscented Transformation (UT), which had been introduced by Julier and Uhlmann in 1994 (Julier & Uhlmann, 1994), have become quite popular in non-linear filter theory over the last two decades. The mathematical basics of UT, however, date back approximately 60 years in time (Tyler, 1953) to the so-called Point Estimate Methods. Formulas had been of interest to solve multi-dimensional integration problems over symmetrical regions, e.g., symmetric probability functions (Evans, 1967, 1974). Due to this symmetry, numerical integration techniques can be derived which at best scale linearly to an n-dimensional integration problem. The general basics of PEMs are shortly summarized below following the annotations given in (Tyler, 1953; Lerner, 2002).

In Point Estimate Methods, the fundamental idea is to choose sample points, ξ_i, and associated weights, w_i, in relation to the first raw moments of the random input variable, ξ. Here, the so-called Generator Function, $GF[\cdot]$, (Tyler, 1953; Lerner, 2002) is of vital importance. A GF describes how sample points are directly determined in $\mathcal{R}^n$ by permutation and the change of sign-combinations. For instance, the first three GFs are illustrated with a problem in $\mathcal{R}^3$:

$$GF[0] = \{(0,0,0)^T\} \tag{11}$$

$$\begin{aligned} GF[\pm\vartheta] = \{&(\vartheta,0,0)^T,\ (-\vartheta,0,0)^T,\ (0,\vartheta,0)^T,\\ &(0,-\vartheta,0)^T,\ (0,0,\vartheta)^T,\ (0,0,-\vartheta)^T\} \end{aligned} \tag{12}$$

$$\begin{aligned} GF[\pm\vartheta,\pm\vartheta] = \{&(\vartheta,\vartheta,0)^T,\ (-\vartheta,-\vartheta,0)^T,\ (\vartheta,-\vartheta,0)^T,\\ &(-\vartheta,\vartheta,0)^T,\ (\vartheta,0,\vartheta)^T,\ (-\vartheta,0,-\vartheta)^T,\\ &(\vartheta,0,-\vartheta)^T,\ (-\vartheta,0,\vartheta)^T,\ (0,\vartheta,\vartheta)^T,\\ &(0,-\vartheta,-\vartheta)^T,\ (0,\vartheta,-\vartheta)^T,\ (0,-\vartheta,\vartheta)^T\} \end{aligned} \tag{13}$$

Here, the scalar parameter, ϑ, controls the spread of the sample points, ξ_i, in $\mathcal{R}^n$. Generally, for the purpose of solving a n-dimensional integration problem, the idea is to use a weighted superposition of function evaluations at GF-based sample points, $g(\xi_i)$, according to

$$\begin{aligned} \int_{\Omega} g(\xi) pdf_{\xi} d\xi \approx w_0 g(GF[0]) + w_1 \sum g(GF[\pm\vartheta]) + \ldots + \\ w_n \sum g(GF[\underbrace{\pm\vartheta,\pm\vartheta,\ldots,\pm\vartheta}_{n \text{ times}}]) \end{aligned} \tag{14}$$

In practical applications, however, a balance has to be found between the total number of used sample points and the resulting precision in calculation. As only a finite number of raw moments of the input random variable, ξ, is considered, the transfer function, $g(\cdot)$, is approximated by monomials of finite degree (Evans, 1967; Lerner, 2002). For instance, by taking account for the first two non-zero raw moments of ξ (still assuming a standard Gaussian distribution), the related monomials of the transfer function, $g(\cdot)$, are $g(\xi) = 1$ and $g(\xi) = \xi[i]^2$ (any element of the random vector, $i \in \{1, \ldots, n\};\ \xi \in \mathcal{R}^n$, could be evaluated due to symmetry, $\xi[i] = \xi[j] \sim \mathcal{N}(0, 1);\ i, j \in \{1, \ldots, n\};\ \xi \in \mathcal{R}^n$). Thus, the transfer function is approximated correctly for monomials of order three. This approximation scheme is labeled as PEM3 in what follows. Remember that any odd power term is zero in association to Gaussian distributions. In this particular case, only the first two Generator Functions, $GF[0] \cap GF[\pm\vartheta]$, can be parametrized by solving the following equation system

$$w_0 + 2nw_1 = \int_\Omega 1 pdf_\xi d\xi = 1 \tag{15}$$

$$2w_1\vartheta^2 = \int_\Omega \xi[i]^2 pdf_\xi d\xi = 1 \tag{16}$$

In consequence, for $\vartheta \neq 0$, the related weights can be calculated via

$$w_0 = 1 - \frac{n}{\vartheta^2} \tag{17}$$

$$w_1 = \frac{1}{2\vartheta^2} \tag{18}$$

As shown in (Julier & Uhlmann, 2004) higher-order moments of the analyzed PDF can be used for the quantification of ϑ additionally. For instance, considering the 4'th raw moment of the standard Gaussian distribution leads to

$$2w_1\vartheta^4 = \int_\Omega \xi[i]^4 pdf_\xi d\xi = 3 \tag{19}$$

Therefore, applying $\vartheta = \sqrt{3}$ might be an optimal choice in case that the probability distribution of η is close to the normal distribution, but different values might be appropriate as well depending on the problem at hand.

After a proper selection of points, $\eta_i = g(\xi_i)$, and associated weights, w_0 & w_1, the mean and the variance of η can be determined approximatively according to

$$E[\eta] \approx \overline{\eta} = w_0\eta_0 + w_1 \sum_{i=1}^{2n} \eta_i \tag{20}$$

$$\begin{aligned}\sigma^2(\eta) \approx\ & w_0(\eta_0 - \overline{\eta})(\eta_0 - \overline{\eta})^T + \\ & w_1 \sum_{i=1}^{2n} (\eta_i - \overline{\eta})(\eta_i - \overline{\eta})^T\end{aligned} \tag{21}$$

In the same manner also higher order moments of η can be approximated according to

$$\begin{aligned}\mu_3 \approx\ & w_0(\eta_0 - \overline{\eta})(\eta_0 - \overline{\eta})^T(\eta_0 - \overline{\eta}) + \\ & w_1 \sum_{i=1}^{2n} (\eta_i - \overline{\eta})(\eta_i - \overline{\eta})^T(\eta_0 - \overline{\eta})\end{aligned} \tag{22}$$

$$\begin{aligned}\mu_4 \approx\ & w_0(\eta_0 - \overline{\eta})(\eta_0 - \overline{\eta})^T(\eta_0 - \overline{\eta})(\eta_0 - \overline{\eta})^T + \\ & w_1 \sum_{i=1}^{2n} (\eta_i - \overline{\eta})(\eta_i - \overline{\eta})^T(\eta_0 - \overline{\eta})(\eta_0 - \overline{\eta})^T\end{aligned} \tag{23}$$

Naturally, the general precision of the PEM approach can be increased gradually by considering higher order raw moments of ξ. For instance, an approximation scheme can be applied which represents monomials of $g(\cdot)$ correctly up to the precision of 5 via

$$\begin{aligned}E[g(\xi)] = \int_\Omega g(\xi) pdf_\xi d\xi \approx\ & w_0 g(GF[0]) + \\ & w_1 g(GF(\pm\vartheta)) + w_2 g(GF(\pm\vartheta, \pm\vartheta))\end{aligned} \tag{24}$$

This approximation scheme is labeled as PEM5 subsequently. In this case, the number of generated sample points, ξ_i, correlates to $2n^2 + 1$ for a n-dimensional integration problem. Here, for the purpose of parametrization of w_i and ϑ an equation system can be derived taking into account monomials of degree 5 or less

$$w_0 + 2nw_1 + 2n(n-1)w_2 = \int 1 pdf_\xi d\xi = 1 \tag{25}$$

$$2w_1\vartheta^2 + 4(n-1)w_2\vartheta^2 = \int \xi[i]^2 pdf_\xi d\xi = 1 \tag{26}$$

$$2w_1\vartheta^4 + 4(n-1)w_2\vartheta^4 = \int \xi[i]^4 pdf_\xi d\xi = 3 \tag{27}$$

$$4w_2\vartheta^4 = \int \xi[i]^2 \xi[j \neq i]^2 pdf_\xi d\xi = 1 \tag{28}$$

Therefore, the four unknowns can be uniquely determined by

the previous equation system as

$$\vartheta = \sqrt{3} \quad (29)$$

$$w_0 = 1 + \frac{n^2 - 7n}{18} \quad (30)$$

$$w_1 = \frac{4 - n}{18} \quad (31)$$

$$w_2 = \frac{1}{36} \quad (32)$$

Obviously, in case of an 1-dimensional input problem, $\xi \in \mathcal{R}^1$, the PEM3 and PEM5 scheme become equivalent for $\vartheta = \sqrt{3}$. In this very special constellation the PEM3 scheme has the same precision as PEM5. This might be one reason why the approximation potential of PEM3 is sometimes overrated in n-dimensional input problems. Alternatively, the following considerations may provide an assessment of the associated approximation power in a readily comprehensible manner.

First, the Eq. (21) is reformulated according to

$$\sigma_\eta^2 \approx \left(w_0 g(\xi_0)^2 + w_1 \sum_{i=1}^{2n} g(\xi_i)^2 \right) - \overline{g}(\xi)^2 \quad (33)$$

$$\sigma_\eta^2 \approx \overline{g(\xi)^2} - \overline{g}(\xi)^2 \quad (34)$$

Obviously, by calculating the variance, σ_η^2, any sample-based approach has to provide a good approximation of $g(\cdot)$ - but of $g(\cdot)^2$, too. Here, the Taylor expansion is in favor as it is sufficient to represent $g(\cdot)$ appropriately. This issue is illustrated in Fig.(1) by an generic 2-dimensional problem, $g(\xi) = \xi[1]^{c_1}\xi[2]^{c_2}$. In case of, $g(\xi)^2 = \xi[1]^{2c_1}\xi[2]^{2c_2}$, monomials of order 4 and higher show up for $c_i > 1, \ \forall i = 1, 2$. Thus, the application of PEM3, which is correct up to monomials of order 3, suffers in precision. In summary, only the PEM5 scheme outperforms the 2. Order Taylor expansion for multi-dimensional input problems and is applied in subsequent considerations for this very reason. (Technical Remark: The same is true when applying PEM3 and PEM5 as an inherent part of Kalman Filtering. Only PEM5 is likely to outperform a so-called second-order Extended Kalman Filter.)

3.1. Non-Gaussian Inputs

So far only the standard Gaussian distribution has been considered. In principle, the PEM concept can be applied for any symmetric distribution. That means, distribution specific sample points and weights can be determined by adapting Eq. (15)-(16) and Eq. (25)-(28), respectively.

In most practical applications, however, one is usually interested in an easy to implement, robust, as well as efficient algorithm. Therefore, a more practicable framework might be desirable. Instead of adapting the weights and sample points according to the distribution at hand, $pdf_{\xi'}$, a (non)-linear transfer function can be derived, $q(\cdot)$, which renders a standard Gaussian distribution into the desired distribution, $\xi' = q(\xi)$. Here, the inverse Rosenblatt transformation (Lee & Chen, 2007) is applied to represent given PDFs associated to ξ' by random variables of standard Gaussian distributions, ξ. Generally, the transformation can be expressed by

$$\xi' = q(\xi) = F^{-1}\left(\Phi(\xi)\right) \quad (35)$$

Here, $F^{-1}(\cdot)$ represents the inverse of the cumulative distribution function (CDF) of the desired random variable ξ', and $\Phi(\cdot)$ denotes the CDF of the standard Gaussian random variable ξ. In the same manner even correlated random variables can be transformed into independent standard Gaussian representatives (Mandur & Budman, 2012). Moreover, empirical (data driven) probability density functions might be incorporated as well, see (Schöniger, Nowak, & Franssen, 2012) for details. In conclusion, the PEM becomes applicable for correlated non-Gaussian random variables. For example, in Tab. 1 some resulting transformation functions are given for frequently used PDFs. Additional transformation formulas can be found in (Isukapalli, 1999).

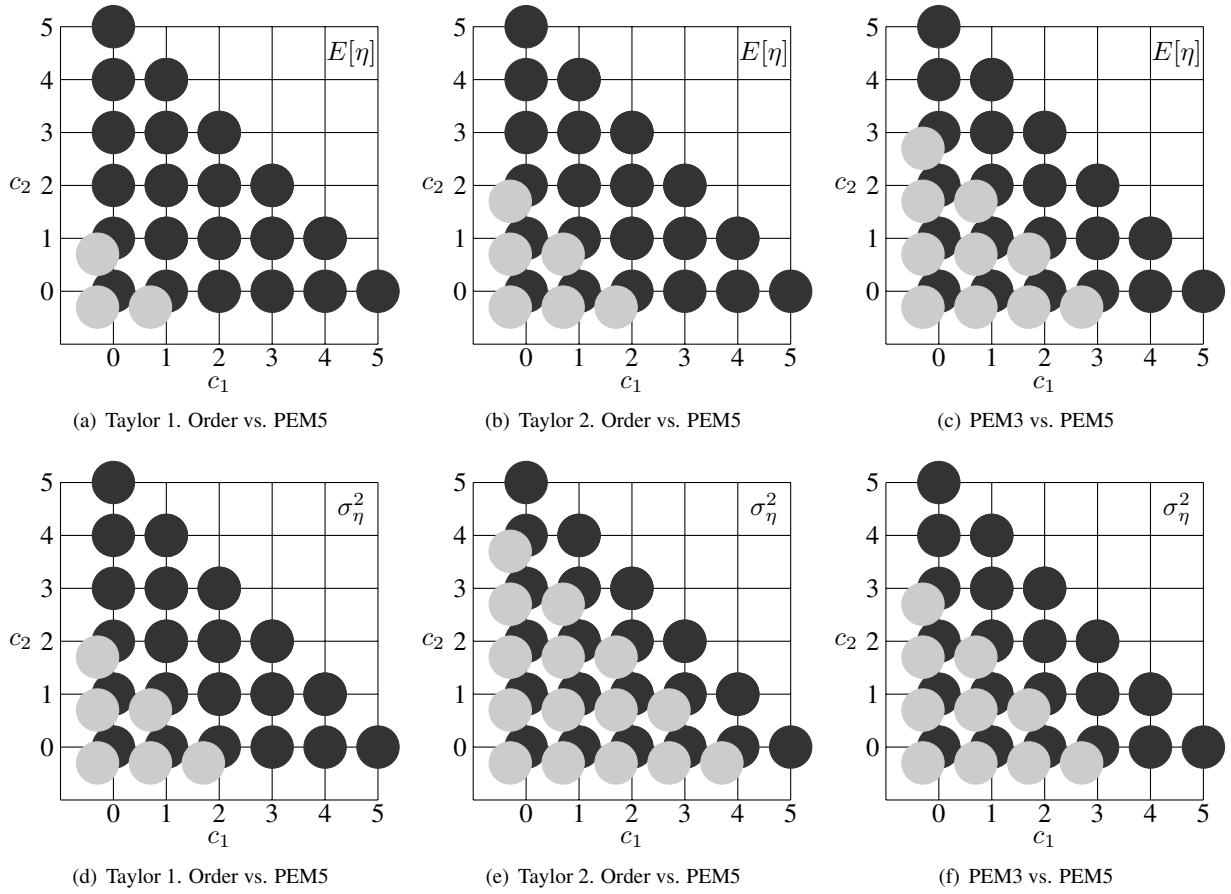
Type of $pdf_{\xi'}$	Transformation: $q(\xi) =$
Normal(μ, σ)	$\mu + \sigma\xi$
Uniform(a, b)	$a + (b-a)\left(\frac{1}{2} + \frac{1}{2}\text{erf}(\xi\sqrt{2})\right)$
Log-normal(μ, σ)	$\exp(\mu + \sigma\xi)$
Gamma(a, b)	$ab\left(\xi\sqrt{\frac{1}{9a}} + 1 - \frac{1}{9a}\right)^3$
Exponential(λ)	$-\frac{1}{\lambda}\log\left(\frac{1}{2} + \frac{1}{2}\text{erf}\left(\frac{\xi}{\sqrt{2}}\right)\right)$

Table 1. Probability density function transformation formulas adapted from (Isukapalli, 1999). Here, the term *erf* means the error function.

Obviously, in most cases, the transformation function, $q(\cdot)$, is a non-linear expression. Hence, as an inherent part of the original uncertainty propagation problem, $\eta = g(q(\xi))$, the overall non-linearity may become more severe. That means, PEMs may suffer in precision to a certain extent additionally. In many practical applications, however, this precision flaw might be acceptable in the light of the easiness in implementation. The numerical results given in Sec. 5 confirm the usefulness of the transformation approach convincingly.

3.2. Non-Gaussian Outputs

The problem of an adequate representation of the resulting output uncertainty, η,is addressed in this subsection. As shown previously, an approximation of the mean, $E[\eta]$, and the vari-



(a) Taylor 1. Order vs. PEM5 (b) Taylor 2. Order vs. PEM5 (c) PEM3 vs. PEM5

(d) Taylor 1. Order vs. PEM5 (e) Taylor 2. Order vs. PEM5 (f) PEM3 vs. PEM5

Figure 1. Benchmark of approximate methods: light gray circles represent the approximation power of the method given in the caption of the sub-figures. Dark gray circles represents the approximation power of PEM5, which is considered as the gold standard. In general, a high number of circles indicates a good approximation power, i.e., the associated monomial, $\eta = \xi[1]^{c_1}\xi[2]^{c_2}$, is approximated correctly. First row is devoted to the mean approximation. Here, the best performance shows the PEM5 approach followed by PEM3, 2. Order Taylor, and, 1. Order Taylor expansion. Second row is devoted to the variance approximation. Here, the best performance shows the PEM5 approach followed by 2. Order Taylor, PEM3, and, 1. Order Taylor expansion.

ance, σ_η^2, can be determined by PEM. Commonly, a Gaussian PDF associated to the simulation result is parameterized by these two quantities. In cases, however, where the actual distribution of η diverges strongly in comparison to a Gaussian PDF misleading inferences might be expected. Here, the additional information of higher order moments of η, e.g., skewness, μ_3, and the kurtosis, μ_4, provided by PEM (Eq. (22)-(23)) might be used as correction factors. For instance, by considering confidence intervals related to η the Cornish-Fisher expansion might be put in operation according to

$$q_p^{cf} = q_p + \frac{(q_p^2-1)\mu_3(\eta)}{6\sigma^3(\eta)} + \frac{(q_p^3-3q_p)\mu_4(\eta)}{24\sigma^4(\eta)} - \frac{(2q_p^3-5q_p)\mu_3^2(\eta)}{36\sigma^6(\eta)} \tag{36}$$

Here, q_p^{cf} is a corrected confidence limit associated to a confidence level p, for more details see (Usaola, 2009) and references therein.

Moreover, the entire PDF of η can be reconstructed efficiently by combining PEM with the Polynomial Chaos Expansion (PCE) concept. In uncertainty analysis, PCE has become quite popular in the last two decades. The essential idea is to represent a random variable, η, by a weighted superposition of an infinity number of basis functions, $\Psi_i(\cdot)$,(Maitre & Knio, 2010) according to

$$\eta = g(\xi) = \sum_{i=0}^{\infty} a_i \Psi_i(\xi) \tag{37}$$

Similar to the Taylor series expansion computational feasibility has to be addressed. Therefore, the expansion in Eq. (37)

is implemented in a truncated form

$$\hat{\eta} = \sum_{i=0}^{l_{pce}} a_i \Psi_i(\xi) \tag{38}$$

By a proper choice of basis functions, $\Psi_i(\cdot)$, the determination of the unknown coefficients, a_i, can be simplified. In particular, different sets of orthogonal basis functions are provided depending on the associated PDF of the random input variable, ξ. For instance, Hermite polynomials are utilized in case of a Gaussian distribution. In literature, different approaches are known to determine the coefficients, a_i, see (Templeton, 2009; Maitre & Knio, 2010) and references therein. Here, the focus is on the least-square approach solely as PEM can be utilized here, too. In practical implementations, a residual, $r(\xi)$, emerges due to the truncation of PCE terms, $l_{pce} << \infty$,

$$r(\xi) = g(\xi) - \sum_{i=0}^{l_{pce}} a_i \Psi_i(\xi) \tag{39}$$

Now, the expected sum of squared errors can be defined as a suitable cost function

$$J_{PCE} = \int_\Omega [r(\xi)]^2 pdf_\xi d\xi \tag{40}$$

The additivity of the expectation operator enables the following reordering

$$J_{PCE} = \int_\Omega g(\xi)^2 pdf_\xi d\xi - 2\int_\Omega g(\xi) \sum_{i=0}^{l_{pce}} a_i \Psi_i(\xi) pdf_\xi d\xi + \int_\Omega \left(\sum_{i=0}^{l_{pce}} a_i \Psi_i(\xi) \right)^2 pdf_\xi d\xi \tag{41}$$

The minimum of this cost function can be found by differentiation of Eq. (41) with respect to a_i, and by setting the resulting derivative equal to zero. Here, due the orthogonality of Ψ_i the mathematical expression results in

$$\frac{\partial J_{PCE}}{\partial a_i} = -2\int_\Omega g(\xi)\Psi_i(\xi) pdf_\xi d\xi + 2a_i \int_\Omega \Psi_i(\xi)^2 pdf_\xi d\xi \stackrel{!}{=} 0 \tag{42}$$

Therefore, the i^{th} coefficient can be calculated according to

$$a_i = \frac{\int_\Omega g(\xi)\ \Psi_i\ pdf_\xi\ d\xi}{\int_\Omega \Psi_i(\xi)^2\ pdf_\xi\ d\xi} \tag{43}$$

In case of Hermite polynomials, the denominator can be determined immediately, see (Maitre & Knio, 2010) for details. The numerator of Eq. (43), however, has to be derived numerically. Obviously, instead of solving one of the original integrals, Eq. (2)-(6), a modified integration problem has to be tackled. Here, a proper quantification of the coefficients, a_i, ensures an optimal parametrization of PCE, Eq. (38). By combining PCE with PEM5 an overall number of $2n^2+1;\ (\xi \in \mathcal{R}^n)$ function evaluations has to be performed. Subsequently, associated moments of $\hat{\eta}$ can be calculated analytically, e.g., the mean and the variance are determined by

$$E[\hat{\eta}] = a_0 \tag{44}$$

$$\sigma^2_{\hat{\eta}} = \sum_{i=1}^{l_{pce}} a_i^2 \int_\Omega \Psi_i(\xi)^2 pdf_\xi d\xi \tag{45}$$

In addition, a PDF approximation of $\hat{\eta}$ can be derived in combination with Monte Carlo simulations and standard Kernel density estimation algorithm which are available in standard computation/statistic tools, e.g., routines available in MATLAB or in *R!*. Please bear in mind that $\hat{\eta}$ is an algebraic expression of ξ, Eq. (38). Therefore, MC simulations based on $\hat{\eta}$ can be performed at low computational costs. In summary, PCE benefits from its versatility and its good convergence behavior, see (Maitre & Knio, 2010) for additional details.

4. GLOBAL SENSITIVITY ANALYSIS

To assess the influence of the uncertain quantities (called inputs in what follows), ξ, on simulation results, $\eta(t)$, related sensitivities have to be analyzed. Whenever the considered inputs are almost certainly known, i.e. the variance of ξ is low, the sensitivities can be determined by a local approach evaluating the Sensitivity Matrix (SM)

$$SM(t_k) = \left. \frac{\partial \eta(t_k)}{\partial \xi} \right|_{\overline{\xi}} \tag{46}$$

Usually, this is not the case and global methods which take the scatter of inputs explicitly into account have to be applied. Variance-based approaches are tailored to cope with this situation well. Hence, treating inputs, ξ, and the output, $\eta(t)$, as random variables, the amount of variance that each element, $\xi[i]$, adds to the variance of the output, $\sigma^2(\eta(t))$, can be quantified.

The ranking of an input $\xi[i]$ is done by the amount of output variance that disappears, if this input $\xi[i]$ is assumed to be known, $\sigma^2(\xi[i]) = 0$. For any input $\xi[i]$, which is assumed

to be known, a conditional variance, $\underset{-i}{\sigma}{}^2(\eta|\xi[i])$, can be determined. Here, the subscript $-i$ indicates that the variance is taken over all inputs other than $\xi[i]$. As $\xi[i]$ itself is a random variable in reality, the expected value of the conditional variance, $\underset{i}{E}\left[\underset{-i}{\sigma}{}^2(\eta|\xi[i])\right]$, has to be determined. Here, the subscript $\underset{i}{E}$ indicates that the expected value is only taken over the input $\xi[i]$. Finally, the output variance, $\sigma^2(\eta)$, can be separated (Saltelli, Ratto, Tarantola, & Campolongo, 2005) into the following two additive terms

$$\sigma^2(\eta) = \underset{i}{\sigma}{}^2(\underset{-i}{E}[\eta|\xi[i]]) + \underset{i}{E}[\underset{-i}{\sigma}{}^2(\eta|\xi[i])] \tag{47}$$

The variance of the conditional expectation, $\underset{i}{\sigma}{}^2(\underset{-i}{E}[\eta|\xi[i]])$, represents the contribution of input $\xi[i]$ to the variance $\sigma^2(\eta)$. The normalized expression in Eq. 48 is known as the first order sensitivity index (Sobol', 1993) and is used in the following for sensitivity analysis.

$$S_i^\eta = \frac{\underset{i}{\sigma}{}^2(\underset{-i}{E}[\eta|\xi[i]])}{\sigma^2(\eta)} \tag{48}$$

The integrals associated to $\sigma^2(\eta)$, $\underset{-i}{E}[\eta|\xi[i]]$, and $\sigma^2(\eta|\xi[i])$ are commonly evaluated by Monte Carlo (MC) simulations (Sobol', 2001). MC simulations, however, come along with a prohibitively computational load. Thus, the PEM methodology is put in operation to reduce the computational demand significantly. In detail, the overall variance, $\sigma^2(\eta)$, is determined by the PEM5. A total number of $2n^2+1$ sample points have to be evaluated and analyzed. Subsequently, the evaluated samples can be reused to calculate the variance of the conditional expectation, $\underset{i}{\sigma}{}^2(\underset{-i}{E}[\eta|\xi[i]])$, immediately. That means, the total number of function evaluations correlates to $2n^2+1$, i.e., PEM5 renders the Global Sensitivity Analysis into a feasible approach which can be applied with a manageable computational effort to real life scenarios. By implementing the proposed strategy, precision demands are fulfilled automatically, i.e., determined variances are related to monomials of precision 5, whereas the expectations are associated to monomials of precision 3.

5. CASE STUDY

The proposed concepts are demonstrated by a generic uncertainty propagation problem according to

$$\eta(t) = g(\xi', t) = \xi'[1]e^{-\xi'[2](e^{-\xi'[3]t})} \tag{49}$$

which may describe the progress in degradation of a technical device. The independent elements of the random vector, ξ', are associated to a non-standard Gaussian, an Uniform, and Log-Normal distribution, respectively. The detail specifications of the applied distributions (Fig. 2) are given by

$$\xi'[1] \sim \mathcal{N}(5, 0.1) \tag{50}$$
$$\xi'[2] \sim \mathcal{U}(1, 3) \tag{51}$$
$$\xi'[3] \sim \ln\mathcal{N}(1, 0.12) \tag{52}$$

By applying feasible transfer functions, $q_i(\cdot)$, the problem of uncertainty propagation is based on standard Gaussian distribution, $\xi[i] \sim \mathcal{N}(0,1);\ \forall i = 1,2,3$, solely:

$$\eta(t) = g(q(\xi), t) = q_1(\xi[1])e^{-q_2(\xi[2])(e^{-q_3(\xi[3])t})} \tag{53}$$

Obviously, by applying PEM5 there is a need for evaluating $g(\cdot)$ 19 times ($\xi \in \mathcal{R}^3,\ 2\cdot 3^2+1 = 19$). In comparison to Monte Carlo simulations (10.000 simulation runs), the proposed PEM5 concept provides working results in approximating the mean and the variance of η by a minimum of computational load. The indirect approach, i.e. deriving PCE first and utilizing its coefficients to represent the first two moments of η, provides similar results with the same computational effort. The numerical outcome is illustrated in Fig. 3(a) and 3(b), respectively.

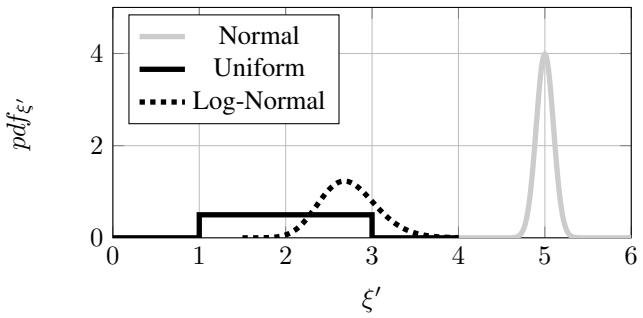
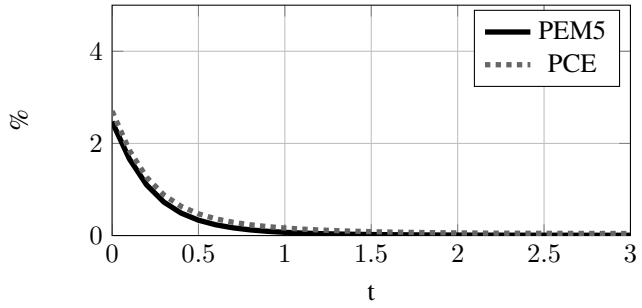
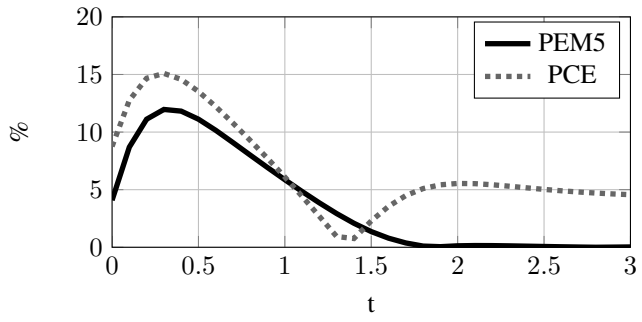


Figure 2. Assumed input uncertainties: $\xi[1]' \sim \mathcal{N}(5, 0.1)$, $\xi[2]' \sim \mathcal{U}(1,3)$, and $\xi[3]' \sim \ln\mathcal{N}(1, 0.12)$.

In principle, with those approximated values confidence intervals, $CI(t) = E[\eta(t)] \pm q_p \cdot \sigma_\eta^2$, can be derived. Due to a potential non-Gaussian distribution associated to η symmetric confidence intervals might lead to misinterpretation in the prognostic framework as indicated by Fig. 4(a). Here, confidence intervals corrected by higher-order statistical moments, i.e. by applying PEM5 and the Cornish-Fisher expansion jointly, might be more credible as demonstrated in Fig. 4(b). Moreover, the indirect approach based on PCE mimics the real uncertainty propagation problem adequately (Fig. 4(c)), too. The entire PDF of $\eta(t)$ might be derived economically by Monte Carlo simulations which evaluate the PCE based surrogate expression, $\hat{g}(\cdot)$, but not a potential CPU-intensive function, $g(\cdot)$. Corresponding snapshots at $t = 0.2$ and $t = 1.0$ are illustrated in Fig. 5 and Fig. 6, respectively.



(a) Approximation error of $E[\eta]$



(b) Approximation error of σ_η^2

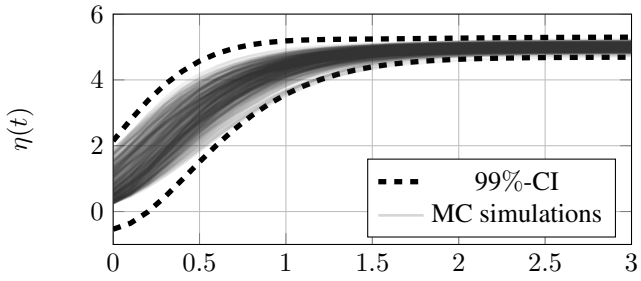
Figure 3. Here, the relative approximation error is illustrated in percentages. PEM5 as well as PCE have an excellent approximation power in relation to the mean, $E[\eta]$. In case of the variance, σ_η^2, PEM5 shows an improved convergence in comparison to PCE.

Here, the non-Gaussian distribution is captured adequately by PCE.

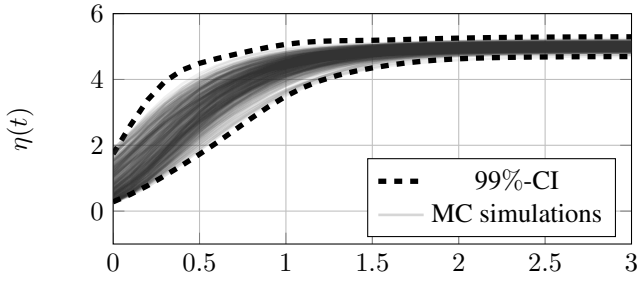
Finally, global sensitivities are analyzed. Assuming the same configuration given in Eq. (50)-(52) the impact of each $\xi[i]$ to the overall variability/uncertainty of $\eta(t)$ is shown in Fig. 7. Here, too, the corresponding Sobol' indices are derived very efficiently. In detail, a total number of $2 \cdot 3^2 + 1 = 19$ function evaluations is sufficient - a remarkable low computational demand in the field of global sensitivity analysis.

6. CONCLUSION

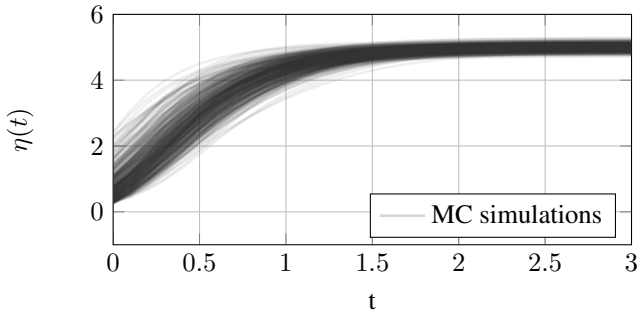
The PEM is identified to be a credible as well as practical concept for the purpose of uncertainty propagation/management. It is demonstrated how PEM can e applied to non-Gaussian distributions by evaluating suitable transfer functions inherently. Moreover, the universal concept of PEM provides an efficient calculation of global sensitivities. Therefore, PEM is a versatile approach which may contribute to tackle an urgent issue in PHM - the reliable propagation of uncertainty in prognostics and health management.



(a) Original PEM5 99%-Confidence Intervals



(b) Cornish-Fisher corrected 99%-Confidence Intervals



(c) PCE based Monte Carlo simulations, i.e., instead of applying $g(\cdot)$ its efficiently to evaluate surrogate $\hat{g}(\cdot)$ is used

Figure 4. Benchmark Monte Carlo simulation vs. approximate concepts. The 99%- CI derived by PEM5 encloses the MC simulations, see (a). The performance can be improved by applying Cornish-Fisher, see (b). Here, the 99%- CI encapsulates the Monte Carlo simulations more reliably. The MC simulations based on PCE (c) fits to original MS simulations given in (a) and (b) quite well.

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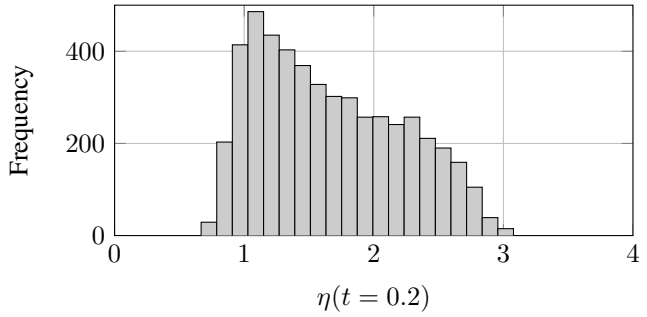
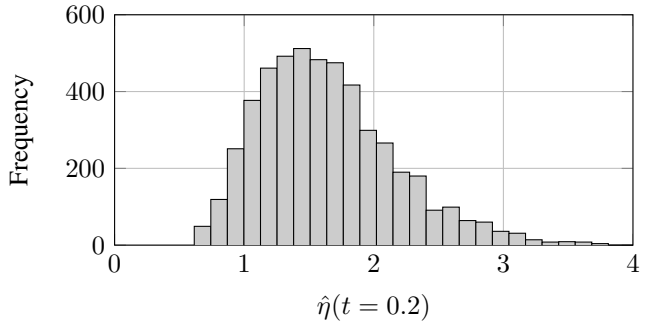
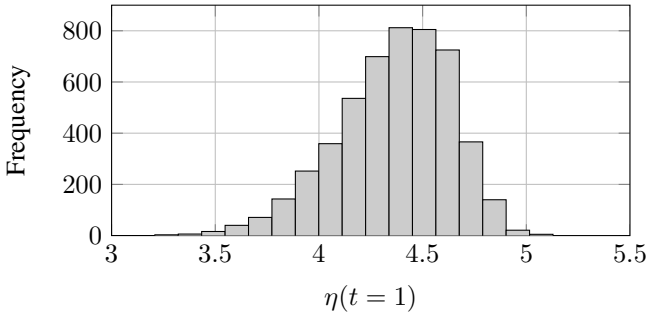


(a) MC simulations based on $g(\cdot)$

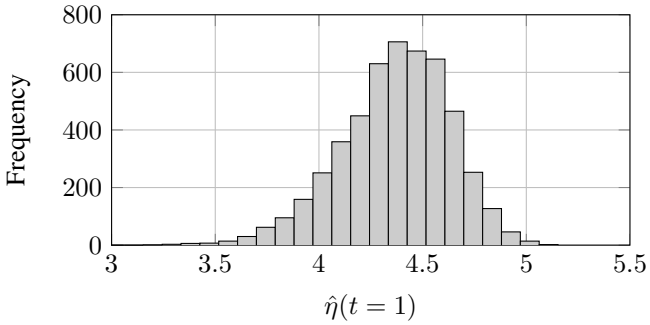


(b) MC simulations based on PCE, $\hat{g}(\cdot)$

Figure 5. Histogram of a snapshot at $t = 0.2$. In (a), the histogram is related to the original evaluation of $g(\cdot)$. In (b), the PCE based surrogate, $\hat{g}(\cdot)$, is evaluated instead. The general characteristics of the distribution are preserved by PCE.



(a) MC simulations based on $g(\cdot)$



(b) MC simulations based on PCE, $\hat{g}(\cdot)$

Figure 6. Histogram of a snapshot at $t = 1$. In (a), the histogram is related to the original evaluation of $g(\cdot)$. In (b), the PCE based surrogate, $\hat{g}(\cdot)$, is evaluated instead. Almost no differences can be detected between sub-figure (a) and (b).

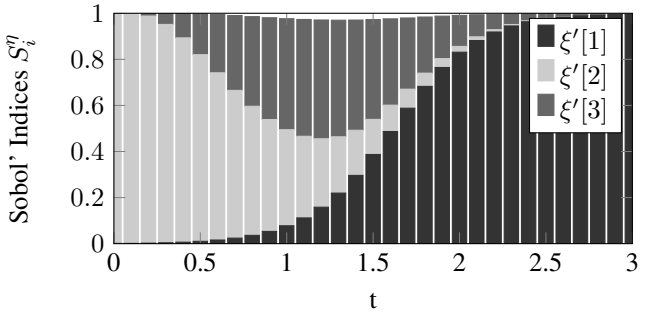


Figure 7. Global parameter sensitivities of $\xi[1]'$,$\xi[2]'$, and $\xi[3]'$ are shown. Obviously, $\xi[2]'$ contributes at most at the very beginning of the simulation. Whereas, $\xi[1]'$ remains the only source of uncertainty at the end of the simulation.

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BIOGRAPHIES

René Schenkendorf received his Dipl.-Ing. in Technical Cybernetics from the Otto-von-Guericke University, Magdeburg in Germany in 2007. From 2007 until 2012 he had been a Ph.D. student at the Max Planck Institute for Dynamics of Complex Technical Systems in Magdeburg, Germany. His dissertation titled "Optimal Experimental Design for Parameter Identification and Model Selection" has been submitted to the Otto-von-Guericke University, Magdeburg, Germany in 2013. The focus in this study was about uncertainty quantification and propagation. Since 2013 he is with the German Aerospace Center at the Institute of Transportation Systems. His current research interests include data analysis, statistical process control, uncertainty propagation, and modeling.

APPENDIX

Following Hermite polynomials have been applied:

$$
\begin{aligned}
\Psi_0(\xi) &= 1 \\
\Psi_1(\xi) &= \xi[1] \\
\Psi_2(\xi) &= \xi[1]^2 - 1 \\
\Psi_3(\xi) &= \xi[1]^3 - 3\xi[1] \\
\Psi_4(\xi) &= \xi[2] \\
\Psi_5(\xi) &= \xi[2]^2 - 1 \\
\Psi_6(\xi) &= \xi[2]^3 - 3\xi[2] \\
\Psi_7(\xi) &= \xi[3] \\
\Psi_8(\xi) &= \xi[3]^2 - 1 \\
\Psi_9(\xi) &= \xi[3]^2 - 3\xi[3] \\
\Psi_{10}(\xi) &= \xi[1]\xi[2] \\
\Psi_{11}(\xi) &= \xi[1]^2\xi[2] - \xi[2] \\
\Psi_{12}(\xi) &= \xi[2]^2\xi[1] - \xi[1] \\
\Psi_{13}(\xi) &= \xi[3] \\
\Psi_{14}(\xi) &= \xi[1]^2\xi[3] - \xi[3] \\
\Psi_{15}(\xi) &= \xi[3]^2\xi[1] - \xi[1] \\
\Psi_{16}(\xi) &= \xi[2]\xi[3] \\
\Psi_{17}(\xi) &= \xi[2]^2\xi[3] - \xi[3] \\
\Psi_{18}(\xi) &= \xi[3]^2\xi[2] - \xi[2] \\
\Psi_{19}(\xi) &= \xi[1]\xi[2]\xi[3]
\end{aligned}
$$

Following coefficients have been utilized:

$$
\begin{aligned}
\int_\Omega \Psi_0(\xi)^2 \; pdf_\xi \; d\xi &= 1 \\
\int_\Omega \Psi_1(\xi)^2 \; pdf_\xi \; d\xi &= 1 \\
\int_\Omega \Psi_2(\xi)^2 \; pdf_\xi \; d\xi &= 2 \\
\int_\Omega \Psi_3(\xi)^2 \; pdf_\xi \; d\xi &= 6 \\
\int_\Omega \Psi_4(\xi)^2 \; pdf_\xi \; d\xi &= 1 \\
\int_\Omega \Psi_5(\xi)^2 \; pdf_\xi \; d\xi &= 2 \\
\int_\Omega \Psi_6(\xi)^2 \; pdf_\xi \; d\xi &= 6 \\
\int_\Omega \Psi_7(\xi)^2 \; pdf_\xi \; d\xi &= 1 \\
\int_\Omega \Psi_8(\xi)^2 \; pdf_\xi \; d\xi &= 2 \\
\int_\Omega \Psi_9(\xi)^2 \; pdf_\xi \; d\xi &= 6 \\
\int_\Omega \Psi_{10}(\xi)^2 \; pdf_\xi \; d\xi &= 1 \\
\int_\Omega \Psi_{11}(\xi)^2 \; pdf_\xi \; d\xi &= 2 \\
\int_\Omega \Psi_{12}(\xi)^2 \; pdf_\xi \; d\xi &= 2 \\
\int_\Omega \Psi_{13}(\xi)^2 \; pdf_\xi \; d\xi &= 1 \\
\int_\Omega \Psi_{14}(\xi)^2 \; pdf_\xi \; d\xi &= 2 \\
\int_\Omega \Psi_{15}(\xi)^2 \; pdf_\xi \; d\xi &= 2 \\
\int_\Omega \Psi_{16}(\xi)^2 \; pdf_\xi \; d\xi &= 1 \\
\int_\Omega \Psi_{17}(\xi)^2 \; pdf_\xi \; d\xi &= 2 \\
\int_\Omega \Psi_{18}(\xi)^2 \; pdf_\xi \; d\xi &= 2 \\
\int_\Omega \Psi_{19}(\xi)^2 \; pdf_\xi \; d\xi &= 1
\end{aligned}
$$